Quantum Chemical Approach to X-ray Spectroscopy: application to small molecules and surfaces

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Modern quantum chemical tools allow us to obtain reliable spectroscopic data for free and adsorbed molecules as well as for local sites at substrate surfaces and in the bulk. The corresponding theoretical results can help to interpret experimental spectra and can provide an understanding of excitation phenomena and other physical behavior on a microscopic scale. This applies, in particular, to electron spectroscopy experiments using synchrotron radiation such as X-ray absorption, XAS/NEXAFS, X-ray emission , XES, and X-ray photoemission, XPS. In this talk we describe quantum chemical methods to evaluate energetics and (angle- resolved) transition matrix elements for photon absorption and emission involving electronically excited states. Our methods are based on modern Density-Functional Theory (DFT) together with gradient corrected functionals as implemented in the StoBe (**Sto**ckholm-**Be**rlin collaboration) code. Approaches and computational strategies will be illustrated by examples of recent theoretical studies on C_6 ring containing hydrocarbons in gas phase and adsorbed at Cu(111), as well as on differently coordinated oxygen in vanadium oxide, V_2O_5 and V_2O_3, in comparison with experiment.